Supporting Information

Molecular Dynamics Simulation Study on CO_2 Physical Absorption Mechanisms for Ethylene-Glycol-Based Solvents Using Free Energy Calculations

Ryo Nagumo[1], Yukihiro Muraki[1], Shuichi Iwata[1], Hideki Mori[1], Hiromitsu Takaba[2], and Hidetaka Yamada[3]*

[1]Department of Materials Science and Engineering, Nagoya Institute of Technology, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan

[2]Department of Environmental Chemistry and Chemical Engineering, Kogakuin University 2665-1 Nakano-machi, Hachioji-shi, Tokyo 192-0015, Japan.

[3]Research Institute of Innovative Technology for the Earth (RITE), 9-2 Kizugawadai, Kizugawa-shi, Kyoto 619-0292, Japan

*Phone: +81-52-735-5214

Table S1. Number of surrounding solvent molecules in the simulation cubic cells, cell lengths, and computational periods for the data sampling in free energy calculations for a CO_2 molecule approaching a solvent molecule in the surrounding solvent molecules.

Solvate–solvent	Number of solvent molecules	Cubic cell length [Å]	Computational period [ns]
CO_2–Glycerol	128	25.1145	1–10
CO_2–EG1	180	25.5414	1–7
CO_2–EG2	128	27.2746	1.5–9
CO_2–DEGDME	83	27.11	1–10
CO_2–EG3	90	27.2588	2–14
CO_2–EG4	61	26.1371	2–20

Table S2. Time steps and computational periods for the data sampling in free energy calculations for a CO_2 molecule approaching a solvent molecule in a vacuum.

Solvate–solvent	Time step [fs]	Computational period [ns]	Solvate–solvent	Time step [fs]	Computational period [ns]
CO_2–EG2	1	1–10	CO_2–EG4-alkane	0.05	0.05–0.5
CO_2–EG2-diol	1	1–10	CO_2–DEGDME	0.5	0.5–5
CO_2–EG2-ether	0.01	0.01–0.1	CO_2–DEGDME-methoxy	0.05	0.05–0.5
CO_2–EG2-alkane	0.01	0.01–0.1	CO_2–DEGDME-ether	0.1	0.1–1
CO_2–EG3	1	1–10	CO_2–DEGDME-alkane	0.1	0.1–1
CO_2–EG3-diol	1	1–10	CO_2–glycerol	1	1–10
CO_2–EG3-ether	0.01	0.01–0.1	CO_2–1,2-butanediol	1	1–10
CO_2–EG3-alkane	0.01	0.01–0.1	CO_2–2-methylpropane-1,3-diol	1	1–10
CO_2–EG4	1	1–10	CO_2–2-methylbutanol	1	1–10
CO_2–EG4-diol	1	1–10	CO_2–3-pentanol	1	1–10
CO_2–EG4-ether	0.05	0.05–0.5	CO_2–3-methylpentane	0.01	0.01–0.1

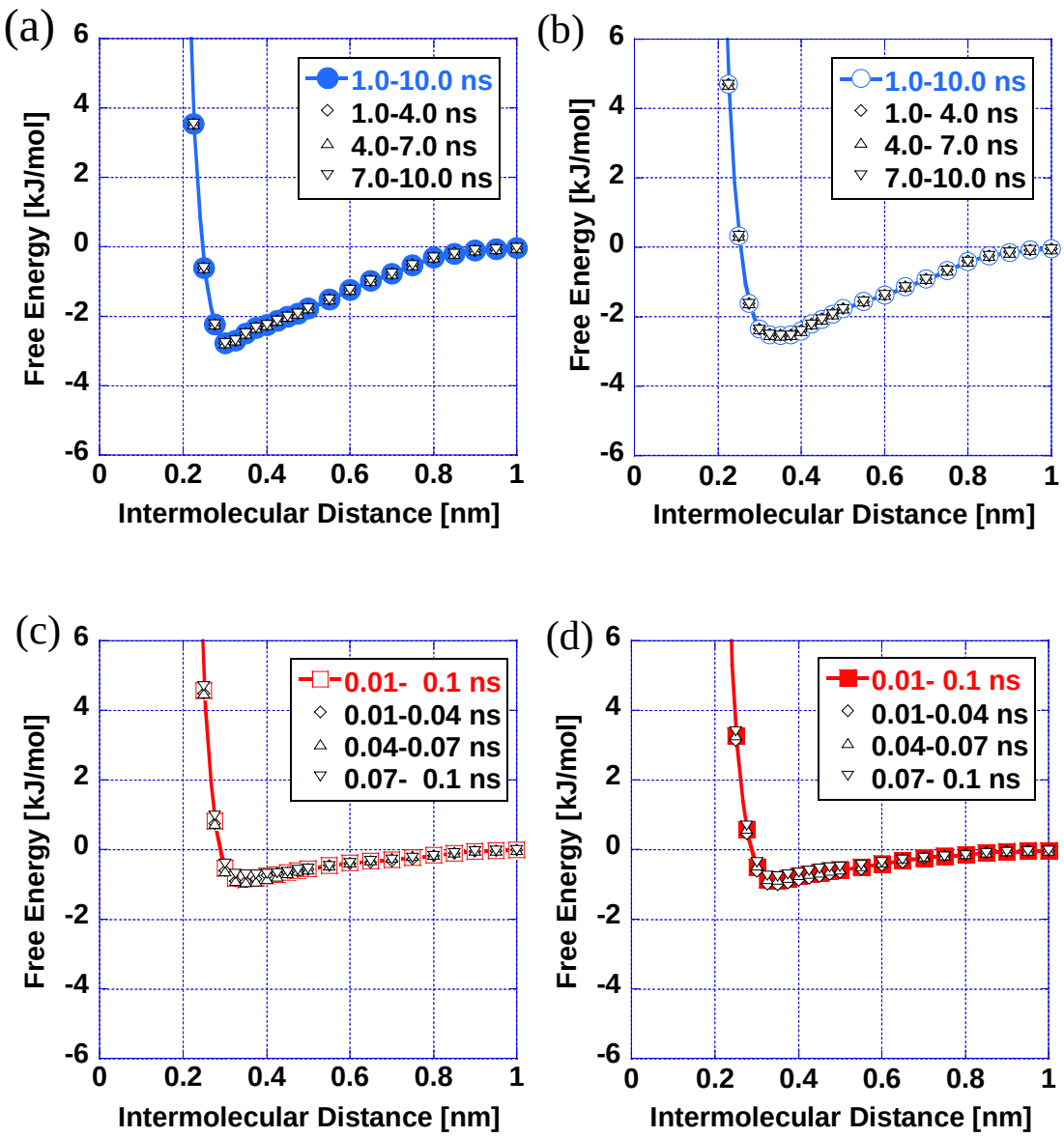

Figure S1. Free energy profiles at 298 K of CO_2 approaching EG2 and the derivative molecules in vacuum: (a) EG2, (b) EG2-diol, (c) EG2-ether, and (d) EG2-alkane.

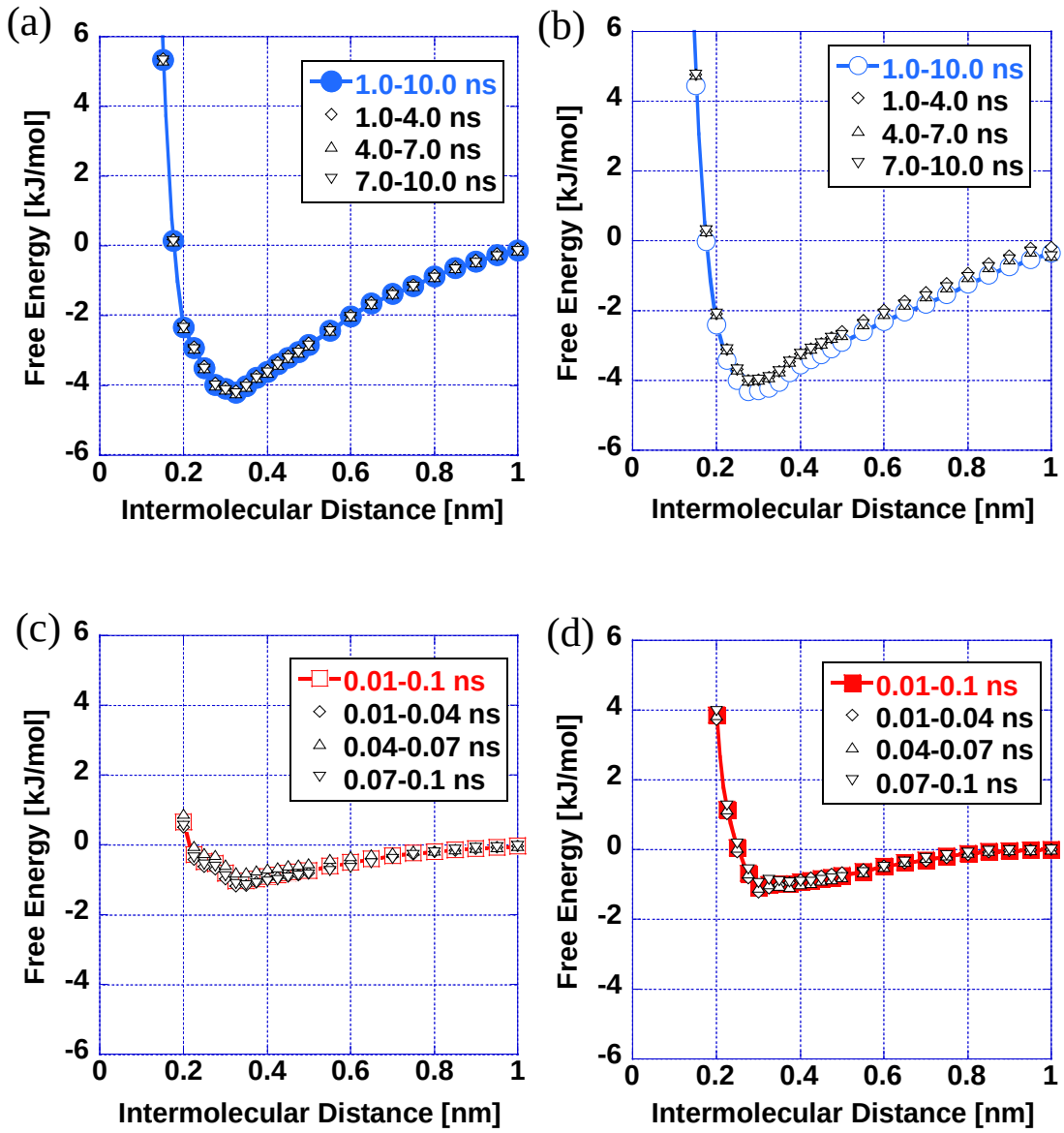

Figure S2. Free energy profiles at 298 K of CO_2 approaching EG3 and the derivative molecules in vacuum: (a) EG3 (reprinted from our previous study[20] with permission from the Society of Chemical Engineers, Japan), (b) EG3-diol, (c) EG3-ether, and (d) EG3-alkane.

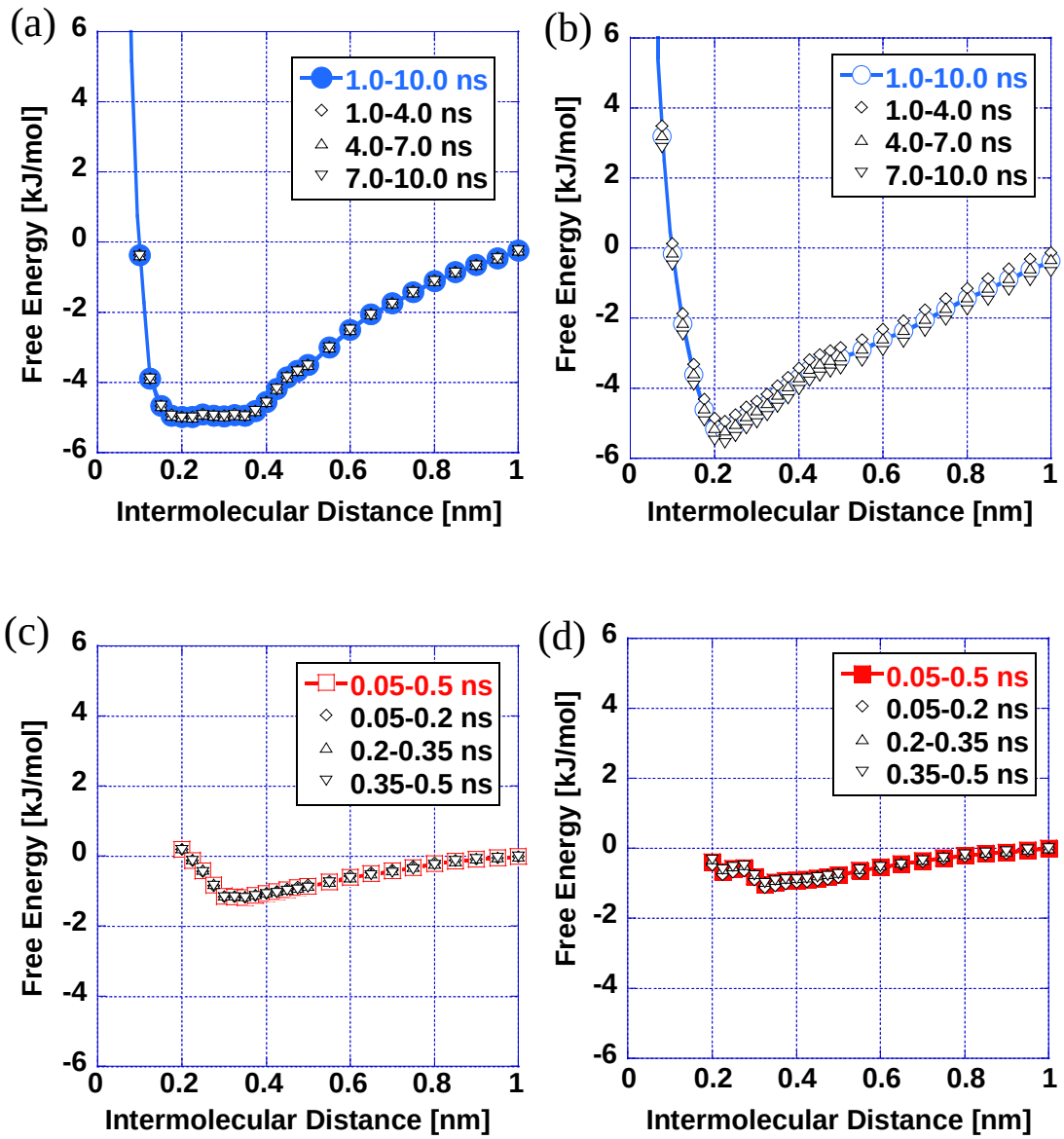

Figure S3. Free energy profiles at 298 K of CO_2 approaching EG4 and the derivative molecules in vacuum: (a) EG4 (reprinted from our previous study[20] with permission from the Society of Chemical Engineers, Japan), (b) EG4-diol, (c) EG4-ether, and (d) EG4-alkane.

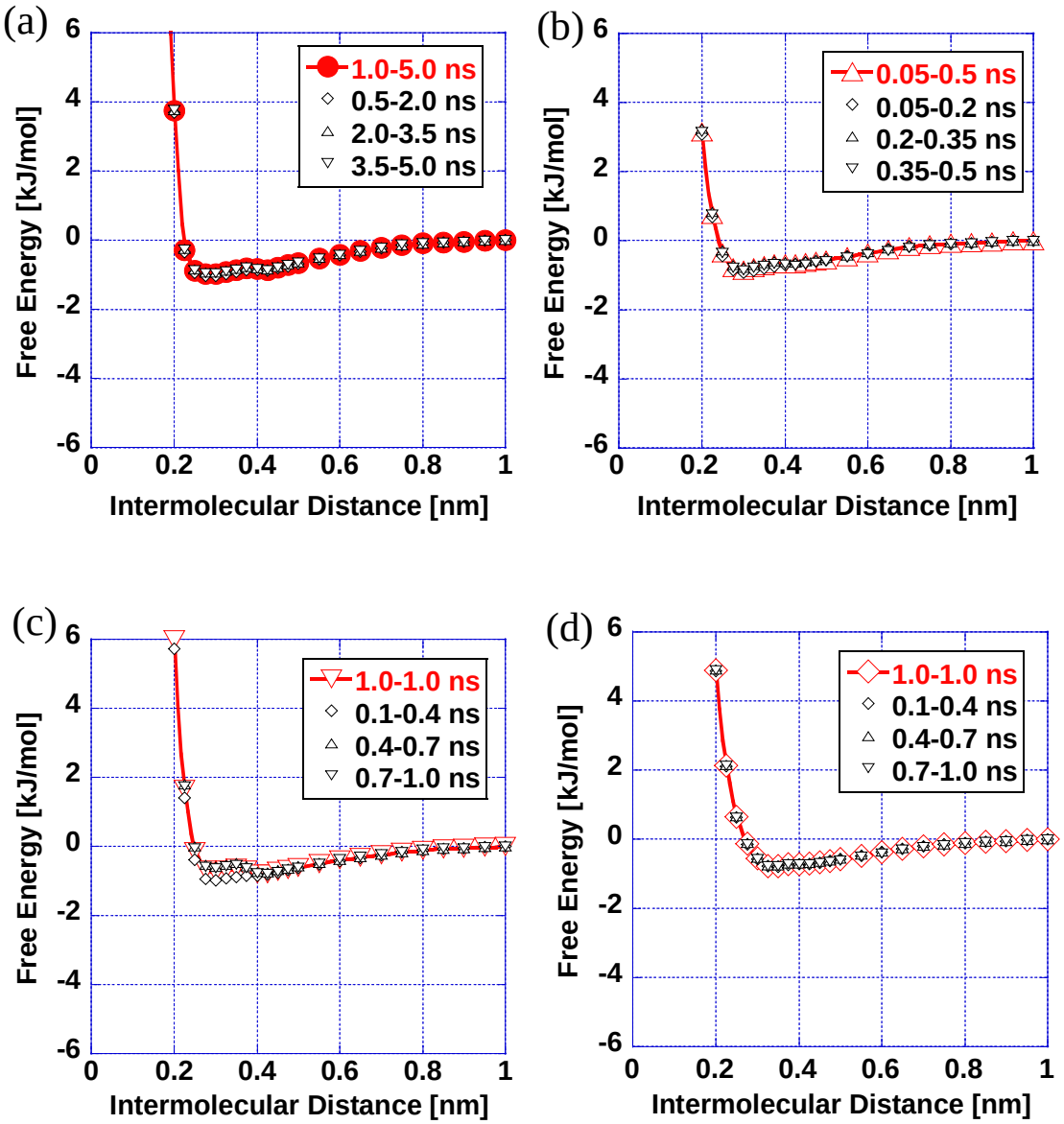

Figure S4. Free energy profiles at 298 K of CO_2 approaching DEGDME and the derivative molecules in vacuum: (a) DEGDME (reprinted from our previous study[20] with permission from the Society of Chemical Engineers, Japan), (b) DEGDME-methoxy, (c) DEGDME-ether, and (d) DEGDME-alkane.

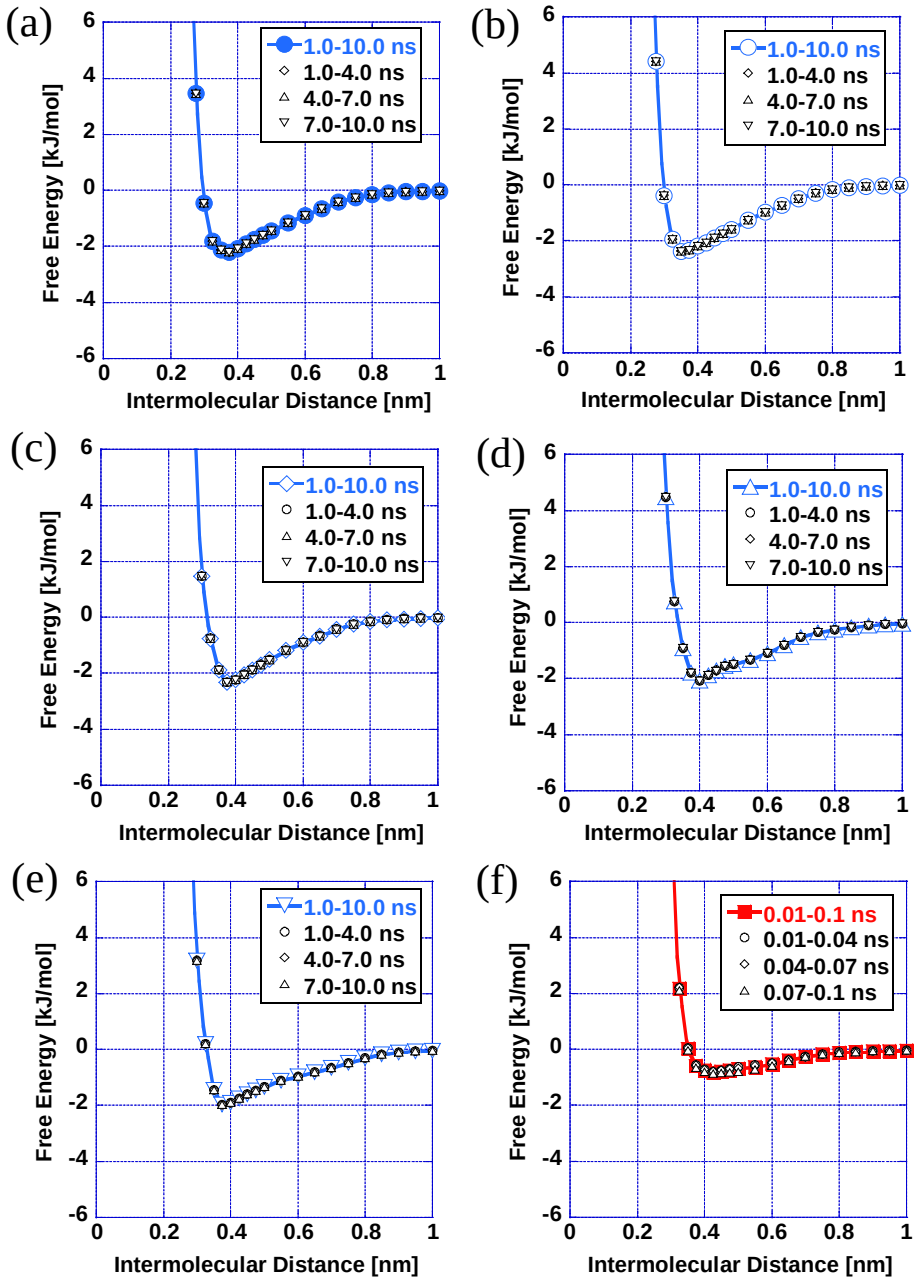

Figure S5. Free energy profiles at 298 K of CO_2 approaching glycerol and the derivative molecules in vacuum: (a) glycerol (reprinted from our previous study[20] with permission from the Society of Chemical Engineers, Japan), (b) 1,2-butanediol, (c) 2-methylpropane-1,3-diol, (d) 2-methylbutanol, (e) 3-pentanol, and (f) 3-methylpentane.